Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 10:09 AM EDT

PDB ID	:	1LPF
Title	:	THREE-DIMENSIONAL STRUCTURE OF LIPOAMIDE DEHYDROGENASE FROM PSEUDOMONAS FLUORESCENS AT 2.8 ANGSTROMS RESOLUTION. ANALYSIS OF REDOX AND THERMOSTABILITY PROPERTIES
Authors	:	Mattevi, A.; Hol, W.
Deposited on	:	1992-10-26
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

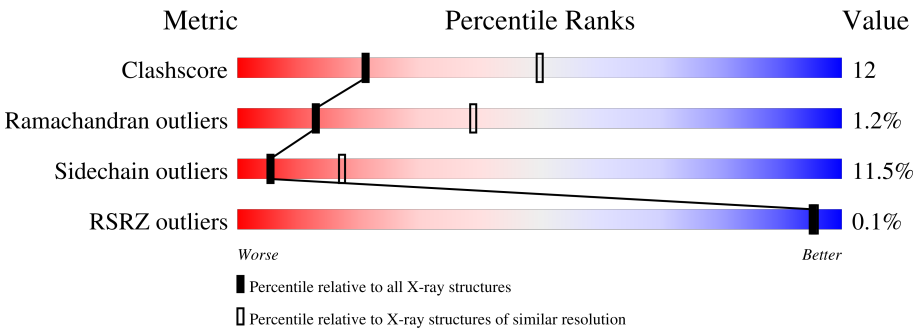
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	477	65% 27% 5% ••
1	B	477	67% 25% 6% ••

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6962 atoms, of which 0 are hydrogens and 0 are deuteriums.

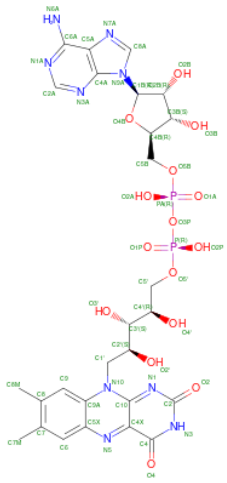
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DIHYDROLIPOAMIDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	472	3428	2172	588	656	12	0	0	0
1	B	472	3428	2172	588	656	12	0	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD



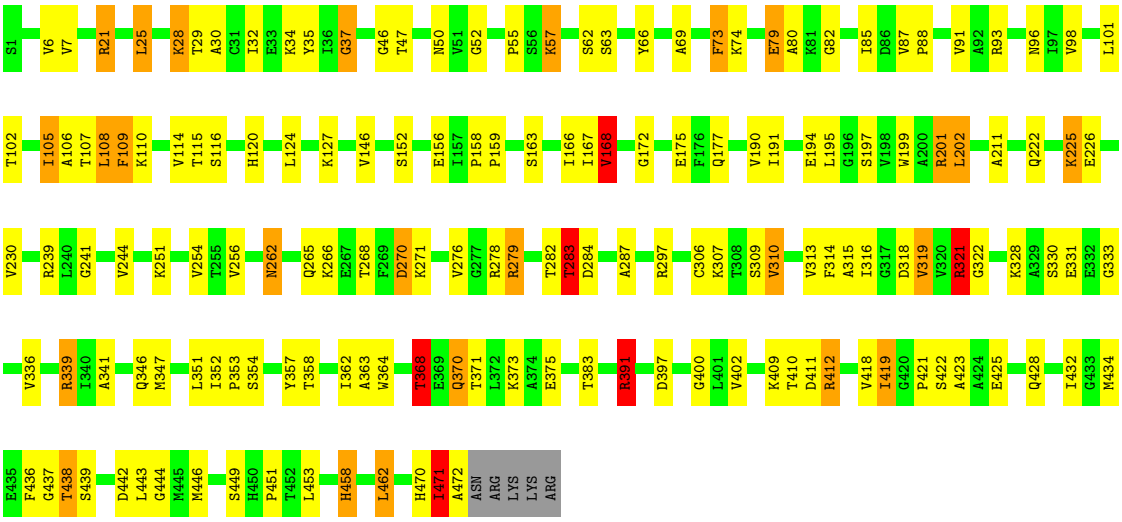
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

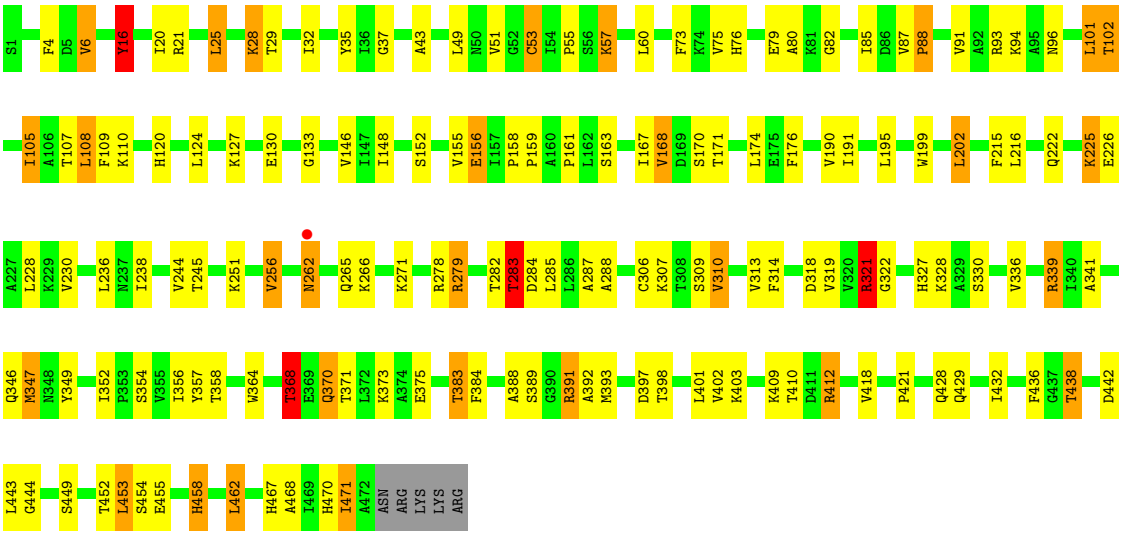
- Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE

Chain A:



- Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	113.60Å 66.40Å 164.30Å 90.00° 99.20° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 15.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.80) 78.8 (15.05-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.22 (at 2.81Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.192 , (Not available) 0.170 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	46.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 64.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6962	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.04	0/3480	1.64	46/4725 (1.0%)
1	B	1.01	2/3480 (0.1%)	1.65	36/4725 (0.8%)
All	All	1.03	2/6960 (0.0%)	1.65	82/9450 (0.9%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	458	HIS	CA-CB	-5.63	1.41	1.53
1	B	453	LEU	CA-CB	-5.14	1.42	1.53

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	339	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	A	391	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	B	278	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	B	321	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	A	434	MET	CG-SD-CE	-8.23	87.04	100.20
1	A	66	TYR	CB-CG-CD2	-8.09	116.14	121.00
1	A	364	TRP	CD1-CG-CD2	8.03	112.73	106.30
1	B	364	TRP	CG-CD2-CE3	7.87	140.99	133.90
1	A	364	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	A	321	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	93	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	B	339	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	397	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	A	278	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	B	364	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	B	364	TRP	CD1-CG-CD2	7.02	111.91	106.30
1	B	391	ARG	NE-CZ-NH1	6.94	123.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	16	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	A	276	VAL	CA-CB-CG2	-6.74	100.78	110.90
1	A	339	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	168	VAL	N-CA-CB	-6.72	96.72	111.50
1	B	155	VAL	CA-CB-CG2	-6.72	100.83	110.90
1	A	98	VAL	CG1-CB-CG2	-6.70	100.17	110.90
1	B	393	MET	CA-CB-CG	-6.65	101.99	113.30
1	A	201	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	199	TRP	CD1-CG-CD2	6.60	111.58	106.30
1	B	368	THR	N-CA-CB	-6.60	97.77	110.30
1	A	279	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	199	TRP	CE2-CD2-CG	-6.52	102.08	107.30
1	B	279	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	199	TRP	CE2-CD2-CG	-6.47	102.13	107.30
1	B	168	VAL	N-CA-CB	-6.45	97.31	111.50
1	B	364	TRP	CB-CG-CD1	-6.39	118.69	127.00
1	B	199	TRP	CD1-CG-CD2	6.36	111.39	106.30
1	B	102	THR	N-CA-CB	-6.34	98.25	110.30
1	A	225	LYS	CA-CB-CG	6.29	127.24	113.40
1	B	278	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	283	THR	CA-C-N	6.24	130.93	117.20
1	A	199	TRP	CG-CD2-CE3	6.22	139.50	133.90
1	A	166	ILE	CG1-CB-CG2	-6.21	97.73	111.40
1	B	283	THR	CA-CB-CG2	6.18	121.05	112.40
1	B	256	VAL	CA-CB-CG2	-6.04	101.84	110.90
1	B	467	HIS	N-CA-C	6.00	127.21	111.00
1	A	102	THR	N-CA-CB	-5.99	98.91	110.30
1	A	270	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	127	LYS	CB-CG-CD	-5.94	96.16	111.60
1	A	251	LYS	CA-CB-CG	5.83	126.23	113.40
1	B	228	LEU	O-C-N	5.80	131.98	122.70
1	A	7	VAL	CG1-CB-CG2	-5.79	101.63	110.90
1	B	397	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	437	GLY	CA-C-O	-5.69	110.36	120.60
1	A	73	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	A	364	TRP	CG-CD2-CE3	5.67	139.00	133.90
1	A	268	THR	O-C-N	-5.58	113.77	122.70
1	A	276	VAL	CA-CB-CG1	5.54	119.20	110.90
1	A	368	THR	N-CA-CB	-5.50	99.84	110.30
1	A	449	SER	CB-CA-C	-5.49	99.67	110.10
1	A	175	GLU	N-CA-CB	-5.39	100.91	110.60
1	A	283	THR	CA-CB-CG2	5.38	119.94	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	239	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	251	LYS	CA-CB-CG	5.34	125.14	113.40
1	A	319	VAL	CB-CA-C	-5.33	101.28	111.40
1	B	306	CYS	CA-CB-SG	-5.32	104.43	114.00
1	A	114	VAL	CA-C-N	-5.31	105.51	117.20
1	A	402	VAL	CG1-CB-CG2	-5.30	102.41	110.90
1	B	236	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	339	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	336	VAL	CG1-CB-CG2	-5.29	102.44	110.90
1	B	109	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	A	270	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	127	LYS	CB-CG-CD	-5.18	98.12	111.60
1	A	412	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	315	ALA	CA-C-N	5.17	128.57	117.20
1	B	336	VAL	CG1-CB-CG2	-5.17	102.63	110.90
1	A	297	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	458	HIS	CG-CD2-NE2	-5.11	99.49	109.20
1	B	283	THR	CA-C-N	5.10	128.43	117.20
1	B	91	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	B	364	TRP	CA-CB-CG	5.07	123.32	113.70
1	B	412	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	362	ILE	CG1-CB-CG2	-5.03	100.33	111.40
1	B	225	LYS	CA-CB-CG	5.03	124.47	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3428	0	3470	92	0
1	B	3428	0	3470	90	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
All	All	6962	0	7002	169	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ASN:H	1:B:262:ASN:HD22	1.12	0.97
1:B:262:ASN:HD22	1:B:262:ASN:N	1.63	0.94
1:A:262:ASN:HD22	1:A:262:ASN:N	1.65	0.93
1:A:262:ASN:H	1:A:262:ASN:ND2	1.69	0.90
1:A:262:ASN:HD22	1:A:262:ASN:H	0.88	0.85
1:B:262:ASN:H	1:B:262:ASN:ND2	1.83	0.76
1:B:146:VAL:HB	1:B:313:VAL:HG22	1.68	0.74
1:B:428:GLN:O	1:B:432:ILE:HG13	1.89	0.73
1:A:438:THR:HG23	1:B:436:PHE:CZ	2.23	0.73
1:A:146:VAL:HB	1:A:313:VAL:HG22	1.69	0.72
1:A:438:THR:HG23	1:B:436:PHE:HZ	1.54	0.71
1:A:436:PHE:CZ	1:B:438:THR:HG23	2.27	0.68
1:A:438:THR:HG21	1:A:443:LEU:HG	1.75	0.67
1:A:80:ALA:HB1	1:B:80:ALA:HB1	1.77	0.66
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.60	0.65
1:A:436:PHE:HZ	1:B:438:THR:HG23	1.62	0.65
1:B:158:PRO:HG2	1:B:159:PRO:HD3	1.79	0.64
1:A:158:PRO:HG2	1:A:159:PRO:HD3	1.81	0.62
1:A:52:GLY:O	1:A:55:PRO:HD2	1.99	0.62
1:B:370:GLN:NE2	1:B:370:GLN:H	1.97	0.62
1:A:88:PRO:HG3	1:A:177:GLN:HG3	1.80	0.62
1:B:35:TYR:HD2	1:B:43:ALA:HB3	1.65	0.62
1:A:310:VAL:HG22	1:A:313:VAL:HB	1.80	0.61
1:B:262:ASN:N	1:B:262:ASN:ND2	2.37	0.60
1:A:438:THR:HG22	1:A:442:ASP:HB2	1.83	0.60
1:A:351:LEU:O	1:A:353:PRO:HD3	2.02	0.59
1:B:347:MET:HG2	1:B:349:TYR:CE2	2.37	0.59
1:A:163:SER:H	1:A:167:ILE:HB	1.69	0.58
1:A:373:LYS:HA	1:A:373:LYS:HE2	1.87	0.56
1:B:307:LYS:HG2	1:B:314:PHE:HE1	1.71	0.56
1:B:87:VAL:HB	1:B:88:PRO:HD3	1.87	0.56
1:A:226:GLU:O	1:A:230:VAL:HG23	2.05	0.56
1:A:421:PRO:HB2	1:A:453:LEU:HD13	1.87	0.56
1:B:373:LYS:HE2	1:B:373:LYS:HA	1.87	0.56
1:A:87:VAL:O	1:A:91:VAL:HG23	2.05	0.56
1:A:322:GLY:HA3	1:A:328:LYS:HE3	1.88	0.56
1:B:310:VAL:HG22	1:B:313:VAL:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:GLN:O	1:A:432:ILE:HG13	2.05	0.56
1:A:368:THR:HG22	1:A:371:THR:OG1	2.06	0.56
1:B:244:VAL:HG13	1:B:256:VAL:HG13	1.87	0.56
1:B:438:THR:HG22	1:B:442:ASP:HB2	1.88	0.55
1:A:28:LYS:HZ1	1:A:29:THR:H	1.53	0.55
1:B:438:THR:HG21	1:B:443:LEU:HG	1.88	0.55
1:A:244:VAL:HG13	1:A:256:VAL:HG13	1.88	0.55
1:B:444:GLY:O	1:B:458:HIS:HE1	1.89	0.54
1:B:51:VAL:CG1	1:B:171:THR:HG23	2.38	0.54
1:B:124:LEU:HD23	1:B:287:ALA:HB2	1.89	0.54
1:B:120:HIS:HE1	1:B:284:ASP:O	1.91	0.53
1:B:4:PHE:HD1	1:B:28:LYS:HG3	1.74	0.52
1:B:55:PRO:HB3	1:B:94:LYS:HD2	1.90	0.52
1:B:347:MET:HG2	1:B:349:TYR:CZ	2.45	0.52
1:A:370:GLN:NE2	1:A:370:GLN:H	2.07	0.52
1:A:316:ILE:HD12	1:A:333:GLY:HA2	1.92	0.50
1:B:368:THR:HG22	1:B:371:THR:OG1	2.12	0.50
1:B:384:PHE:CZ	1:B:388:ALA:HB3	2.47	0.50
1:A:87:VAL:HB	1:A:88:PRO:HD3	1.92	0.50
1:B:163:SER:H	1:B:167:ILE:HB	1.77	0.49
1:B:191:ILE:O	1:B:195:LEU:HD23	2.12	0.49
1:A:106:ALA:O	1:A:109:PHE:HB2	2.12	0.49
1:A:34:LYS:NZ	1:A:120:HIS:HD2	2.10	0.49
1:B:35:TYR:CD2	1:B:43:ALA:HB3	2.46	0.49
1:B:148:ILE:HG21	1:B:285:LEU:HD21	1.92	0.49
1:B:391:ARG:HH11	1:B:391:ARG:HG3	1.78	0.48
1:A:411:ASP:O	1:A:439:SER:HA	2.14	0.48
1:B:105:ILE:HA	1:B:108:LEU:HB2	1.96	0.48
1:A:438:THR:CG2	1:B:436:PHE:HZ	2.26	0.48
1:A:120:HIS:HE1	1:A:284:ASP:O	1.97	0.48
1:B:156:GLU:HB2	1:B:279:ARG:HH22	1.79	0.48
1:A:339:ARG:HH21	1:A:346:GLN:NE2	2.12	0.48
1:A:30:ALA:HA	1:A:115:THR:O	2.15	0.47
1:A:93:ARG:HD3	1:B:75:VAL:O	2.14	0.47
1:B:322:GLY:HA3	1:B:328:LYS:HE3	1.96	0.47
1:A:25:LEU:HG	1:A:341:ALA:CB	2.45	0.47
1:B:226:GLU:O	1:B:230:VAL:HG23	2.15	0.47
1:B:32:ILE:HG22	2:B:480:FAD:H2A	1.96	0.47
1:B:60:LEU:HD13	1:B:357:TYR:O	2.14	0.47
1:A:57:LYS:HD3	1:A:57:LYS:HA	1.71	0.47
1:B:215:PHE:CE2	1:B:216:LEU:HD12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:SER:HB3	1:B:76:HIS:HB3	1.97	0.46
1:A:74:LYS:HE3	1:A:79:GLU:OE2	2.13	0.46
1:B:421:PRO:HB2	1:B:453:LEU:HD13	1.97	0.46
1:A:211:ALA:O	1:A:241:GLY:HA2	2.16	0.46
1:A:307:LYS:HG2	1:A:314:PHE:HE1	1.81	0.46
1:B:371:THR:O	1:B:375:GLU:HG3	2.16	0.46
1:A:262:ASN:N	1:A:262:ASN:ND2	2.39	0.45
1:A:425:GLU:HG3	1:B:454:SER:OG	2.16	0.45
1:B:191:ILE:HG22	1:B:195:LEU:HD23	1.98	0.45
1:A:57:LYS:HD2	1:A:357:TYR:CG	2.52	0.45
1:B:462:LEU:HB3	1:B:468:ALA:HA	1.99	0.45
1:B:470:HIS:O	1:B:471:ILE:HG23	2.16	0.45
1:A:339:ARG:NH2	1:A:346:GLN:HE22	2.14	0.45
1:B:158:PRO:O	1:B:161:PRO:HG3	2.16	0.45
1:B:410:THR:HG21	1:B:412:ARG:NH2	2.32	0.45
1:A:432:ILE:CD1	1:B:429:GLN:HB3	2.47	0.45
1:B:6:VAL:HB	1:B:29:THR:HG23	1.98	0.45
1:B:53:CYS:O	1:B:57:LYS:HE2	2.16	0.45
1:A:470:HIS:O	1:A:471:ILE:HG23	2.17	0.45
1:B:120:HIS:CE1	1:B:284:ASP:O	2.69	0.45
1:A:354:SER:O	1:A:363:ALA:HA	2.16	0.45
1:B:16:TYR:O	1:B:20:ILE:HG13	2.17	0.45
1:B:170:SER:HB3	2:B:480:FAD:HM71	1.98	0.45
1:A:190:VAL:O	1:A:194:GLU:HG3	2.16	0.44
1:A:28:LYS:HZ2	1:A:28:LYS:HA	1.82	0.44
1:A:444:GLY:O	1:A:458:HIS:HE1	2.00	0.44
1:B:49:LEU:HD21	1:B:101:LEU:HB3	1.99	0.44
1:B:57:LYS:HA	1:B:57:LYS:HD3	1.55	0.44
1:B:94:LYS:NZ	1:B:174:LEU:O	2.51	0.44
1:B:190:VAL:HG22	1:B:356:ILE:HG12	2.00	0.44
1:A:152:SER:HB3	1:A:318:ASP:HB3	2.00	0.44
1:A:462:LEU:HD12	1:A:462:LEU:HA	1.82	0.44
1:A:168:VAL:HG22	1:A:172:GLY:HA3	2.00	0.44
1:A:32:ILE:HG22	2:A:480:FAD:H2A	1.99	0.44
1:B:28:LYS:HZ1	1:B:29:THR:H	1.66	0.44
1:A:35:TYR:CE2	1:A:37:GLY:HA2	2.53	0.43
1:B:110:LYS:HA	1:B:110:LYS:HD3	1.88	0.43
1:B:215:PHE:HE1	1:B:238:ILE:HD13	1.83	0.43
1:A:202:LEU:HD23	1:A:202:LEU:N	2.33	0.43
1:A:451:PRO:HD3	1:B:53:CYS:HB3	1.99	0.43
1:A:471:ILE:O	1:A:472:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LEU:HD11	1:B:130:GLU:HB2	1.99	0.43
1:A:46:GLY:O	1:A:50:ASN:HB2	2.18	0.43
1:A:105:ILE:HA	1:A:108:LEU:HB2	2.01	0.43
1:B:339:ARG:HH21	1:B:346:GLN:NE2	2.16	0.43
1:B:339:ARG:NH2	1:B:346:GLN:HE22	2.17	0.43
1:A:442:ASP:O	1:A:446:MET:HG3	2.19	0.43
1:A:63:SER:HB3	1:A:202:LEU:HD21	2.01	0.43
1:B:159:PRO:HB3	1:B:245:THR:O	2.18	0.43
1:A:371:THR:O	1:A:375:GLU:HG3	2.18	0.43
1:A:438:THR:HG22	1:A:442:ASP:CB	2.48	0.43
1:A:85:ILE:HG12	1:A:202:LEU:HD13	2.01	0.42
1:A:436:PHE:HZ	1:B:438:THR:CG2	2.28	0.42
1:A:156:GLU:HB2	1:A:279:ARG:HH22	1.84	0.42
1:B:85:ILE:HG12	1:B:202:LEU:CD1	2.48	0.42
1:B:321:ARG:H	1:B:321:ARG:HG3	1.70	0.42
1:A:400:GLY:HA3	1:A:419:ILE:O	2.19	0.42
1:B:176:PHE:CZ	1:B:271:LYS:HG2	2.54	0.42
1:A:306:CYS:SG	1:A:321:ARG:NH2	2.93	0.42
1:B:25:LEU:HG	1:B:341:ALA:CB	2.49	0.42
1:B:402:VAL:HG12	1:B:403:LYS:N	2.34	0.42
1:B:455:GLU:O	1:B:458:HIS:HB3	2.19	0.42
1:B:443:LEU:HA	1:B:443:LEU:HD23	1.76	0.42
1:A:191:ILE:HG22	1:A:195:LEU:HD23	2.01	0.42
1:A:331:GLU:HB3	1:A:347:MET:SD	2.60	0.42
1:A:191:ILE:O	1:A:195:LEU:HD23	2.20	0.41
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.84	0.41
1:B:49:LEU:O	1:B:49:LEU:HG	2.20	0.41
1:A:34:LYS:HZ3	1:A:120:HIS:CD2	2.39	0.41
1:A:197:SER:O	1:A:201:ARG:HD3	2.20	0.41
1:A:421:PRO:HB2	1:A:453:LEU:CD1	2.49	0.41
1:B:383:THR:HG23	1:B:401:LEU:HD12	2.03	0.41
1:A:69:ALA:HA	1:A:73:PHE:CG	2.54	0.41
1:B:51:VAL:HG11	1:B:171:THR:HG23	2.02	0.41
1:B:307:LYS:HG2	1:B:314:PHE:CE1	2.52	0.41
1:B:389:SER:HB3	1:B:392:ALA:HB3	2.02	0.41
1:A:270:ASP:O	1:A:271:LYS:HD2	2.21	0.41
1:A:307:LYS:HG2	1:A:314:PHE:CE1	2.56	0.41
1:A:410:THR:HG21	1:A:412:ARG:NH2	2.35	0.41
1:B:256:VAL:O	1:B:266:LYS:HA	2.20	0.41
1:A:28:LYS:NZ	1:A:29:THR:H	2.17	0.41
1:A:47:THR:O	1:A:52:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:SER:O	1:A:423:ALA:C	2.59	0.41
1:A:21:ARG:HH11	1:A:21:ARG:HD3	1.72	0.41
1:A:256:VAL:O	1:A:266:LYS:HA	2.21	0.41
1:B:28:LYS:HZ2	1:B:28:LYS:HA	1.86	0.41
1:B:152:SER:HB3	1:B:318:ASP:HB3	2.03	0.40
1:B:449:SER:HB2	1:B:452:THR:HG21	2.03	0.40
1:A:432:ILE:HD12	1:B:429:GLN:HB3	2.02	0.40
1:A:124:LEU:HD23	1:A:287:ALA:HB2	2.03	0.40
1:A:110:LYS:NZ	1:A:116:SER:HB2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	470/477 (98%)	439 (93%)	27 (6%)	4 (1%)	17	46
1	B	470/477 (98%)	436 (93%)	27 (6%)	7 (2%)	10	33
All	All	940/954 (98%)	875 (93%)	54 (6%)	11 (1%)	13	39

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	THR
1	B	283	THR
1	A	37	GLY
1	A	82	GLY
1	B	82	GLY
1	B	288	ALA
1	B	37	GLY
1	A	471	ILE
1	B	53	CYS

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Mol	Chain	Res	Type
1	B	471	ILE
1	B	133	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	349/365 (96%)	311 (89%)	38 (11%)	6 19
1	B	349/365 (96%)	307 (88%)	42 (12%)	5 15
All	All	698/730 (96%)	618 (88%)	80 (12%)	5 17

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	21	ARG
1	A	25	LEU
1	A	28	LYS
1	A	57	LYS
1	A	79	GLU
1	A	96	ASN
1	A	101	LEU
1	A	105	ILE
1	A	107	THR
1	A	108	LEU
1	A	109	PHE
1	A	168	VAL
1	A	202	LEU
1	A	222	GLN
1	A	225	LYS
1	A	254	VAL
1	A	262	ASN
1	A	265	GLN
1	A	282	THR
1	A	283	THR

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Mol	Chain	Res	Type
1	A	309	SER
1	A	310	VAL
1	A	319	VAL
1	A	321	ARG
1	A	330	SER
1	A	352	ILE
1	A	358	THR
1	A	368	THR
1	A	370	GLN
1	A	383	THR
1	A	391	ARG
1	A	409	LYS
1	A	418	VAL
1	A	419	ILE
1	A	438	THR
1	A	462	LEU
1	A	471	ILE
1	B	6	VAL
1	B	16	TYR
1	B	21	ARG
1	B	25	LEU
1	B	28	LYS
1	B	57	LYS
1	B	73	PHE
1	B	79	GLU
1	B	88	PRO
1	B	96	ASN
1	B	101	LEU
1	B	102	THR
1	B	105	ILE
1	B	107	THR
1	B	108	LEU
1	B	156	GLU
1	B	168	VAL
1	B	202	LEU
1	B	222	GLN
1	B	225	LYS
1	B	262	ASN
1	B	265	GLN
1	B	282	THR
1	B	283	THR
1	B	309	SER

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Mol	Chain	Res	Type
1	B	310	VAL
1	B	319	VAL
1	B	321	ARG
1	B	327	HIS
1	B	330	SER
1	B	347	MET
1	B	352	ILE
1	B	354	SER
1	B	358	THR
1	B	368	THR
1	B	370	GLN
1	B	383	THR
1	B	398	THR
1	B	409	LYS
1	B	418	VAL
1	B	438	THR
1	B	462	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	222	GLN
1	A	262	ASN
1	A	265	GLN
1	A	346	GLN
1	A	396	ASN
1	A	417	HIS
1	A	429	GLN
1	A	458	HIS
1	B	120	HIS
1	B	222	GLN
1	B	262	ASN
1	B	346	GLN
1	B	417	HIS
1	B	429	GLN
1	B	458	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	B	480	-	53,58,58	1.23	5 (9%)	68,89,89	1.83	21 (30%)
2	FAD	A	480	-	53,58,58	1.18	5 (9%)	68,89,89	1.71	17 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	480	-	-	2/30/50/50	0/6/6/6
2	FAD	A	480	-	-	1/30/50/50	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	480	FAD	C1'-C2'	3.56	1.57	1.52
2	A	480	FAD	C5X-N5	-3.37	1.33	1.39
2	B	480	FAD	C5X-N5	-3.13	1.33	1.39
2	B	480	FAD	C9A-N10	-3.08	1.35	1.41
2	B	480	FAD	O4B-C1B	2.54	1.44	1.41
2	A	480	FAD	C9A-N10	-2.50	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	480	FAD	C10-N10	-2.48	1.31	1.37
2	A	480	FAD	C1'-N10	-2.17	1.42	1.48
2	A	480	FAD	C5A-N7A	-2.10	1.32	1.39
2	B	480	FAD	C10-N10	-2.08	1.32	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	480	FAD	C9-C9A-N10	5.26	128.94	121.84
2	A	480	FAD	C9-C9A-N10	4.87	128.41	121.84
2	A	480	FAD	C4-N3-C2	-4.33	117.64	125.64
2	B	480	FAD	C4-N3-C2	-4.26	117.78	125.64
2	B	480	FAD	O2'-C2'-C1'	4.13	119.79	109.80
2	B	480	FAD	N3A-C2A-N1A	-3.55	123.13	128.68
2	B	480	FAD	C10-N1-C2	3.45	123.81	116.90
2	B	480	FAD	C4A-C5A-N7A	3.35	112.89	109.40
2	A	480	FAD	O2'-C2'-C1'	3.18	117.49	109.80
2	B	480	FAD	C4X-C10-N1	-3.06	117.62	124.73
2	A	480	FAD	O2-C2-N1	-2.93	116.97	121.83
2	A	480	FAD	C10-N1-C2	2.80	122.49	116.90
2	B	480	FAD	C5A-C6A-N1A	-2.76	114.09	120.35
2	B	480	FAD	C9-C9A-C5X	-2.74	114.94	120.11
2	A	480	FAD	C4X-C10-N1	-2.73	118.40	124.73
2	A	480	FAD	N3A-C2A-N1A	-2.71	124.44	128.68
2	A	480	FAD	C4A-C5A-N7A	2.71	112.22	109.40
2	B	480	FAD	C1'-N10-C9A	-2.68	116.04	120.51
2	B	480	FAD	C4X-C4-N3	2.66	119.94	113.19
2	A	480	FAD	C9-C9A-C5X	-2.64	115.13	120.11
2	A	480	FAD	C10-C4X-N5	-2.55	119.45	124.86
2	A	480	FAD	C4X-C4-N3	2.38	119.24	113.19
2	B	480	FAD	N6A-C6A-N1A	2.38	123.51	118.57
2	A	480	FAD	C1'-N10-C9A	-2.36	116.57	120.51
2	B	480	FAD	C1'-C2'-C3'	-2.35	103.21	109.79
2	A	480	FAD	O4B-C1B-C2B	-2.32	103.53	106.93
2	A	480	FAD	C4-C4X-C10	2.32	120.69	116.79
2	B	480	FAD	C10-C4X-N5	-2.32	119.94	124.86
2	A	480	FAD	C5A-C6A-N1A	-2.29	115.16	120.35
2	B	480	FAD	C5X-C9A-N10	-2.25	115.63	117.95
2	B	480	FAD	O4-C4-C4X	-2.24	120.66	126.60
2	A	480	FAD	O4-C4-C4X	-2.18	120.81	126.60
2	B	480	FAD	C9A-N10-C10	2.18	124.16	120.77
2	B	480	FAD	N10-C10-N1	2.18	124.62	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	480	FAD	C2A-N1A-C6A	2.15	122.43	118.75
2	B	480	FAD	C9A-C9-C8	2.14	123.62	119.30
2	B	480	FAD	C4-C4X-C10	2.02	120.19	116.79
2	A	480	FAD	N6A-C6A-N1A	2.01	122.75	118.57

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	480	FAD	O4B-C4B-C5B-O5B
2	B	480	FAD	C3B-C4B-C5B-O5B
2	A	480	FAD	O4B-C4B-C5B-O5B

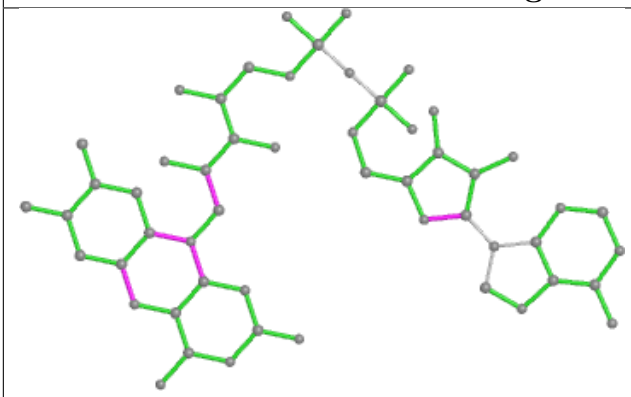
There are no ring outliers.

2 monomers are involved in 3 short contacts:

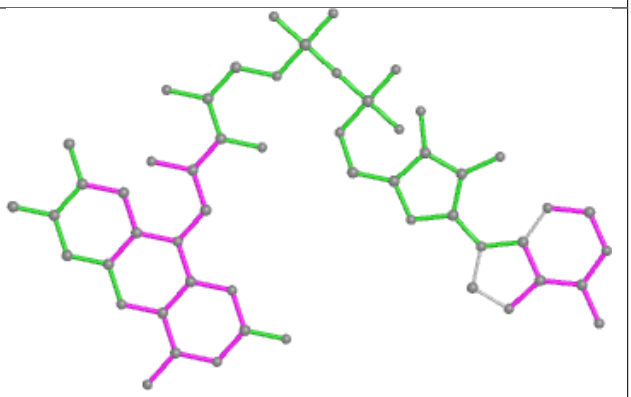
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	480	FAD	2	0
2	A	480	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

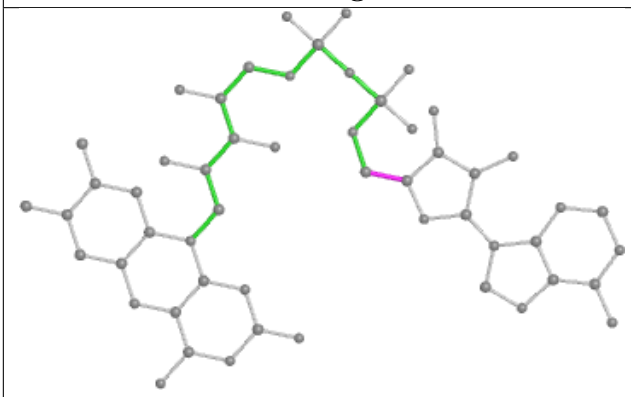
Ligand FAD B 480



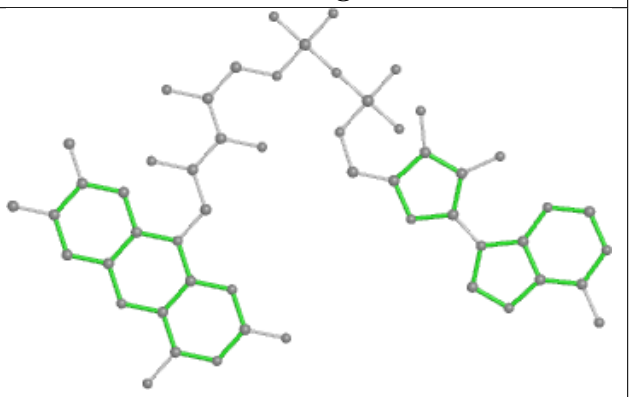
Bond lengths



Bond angles

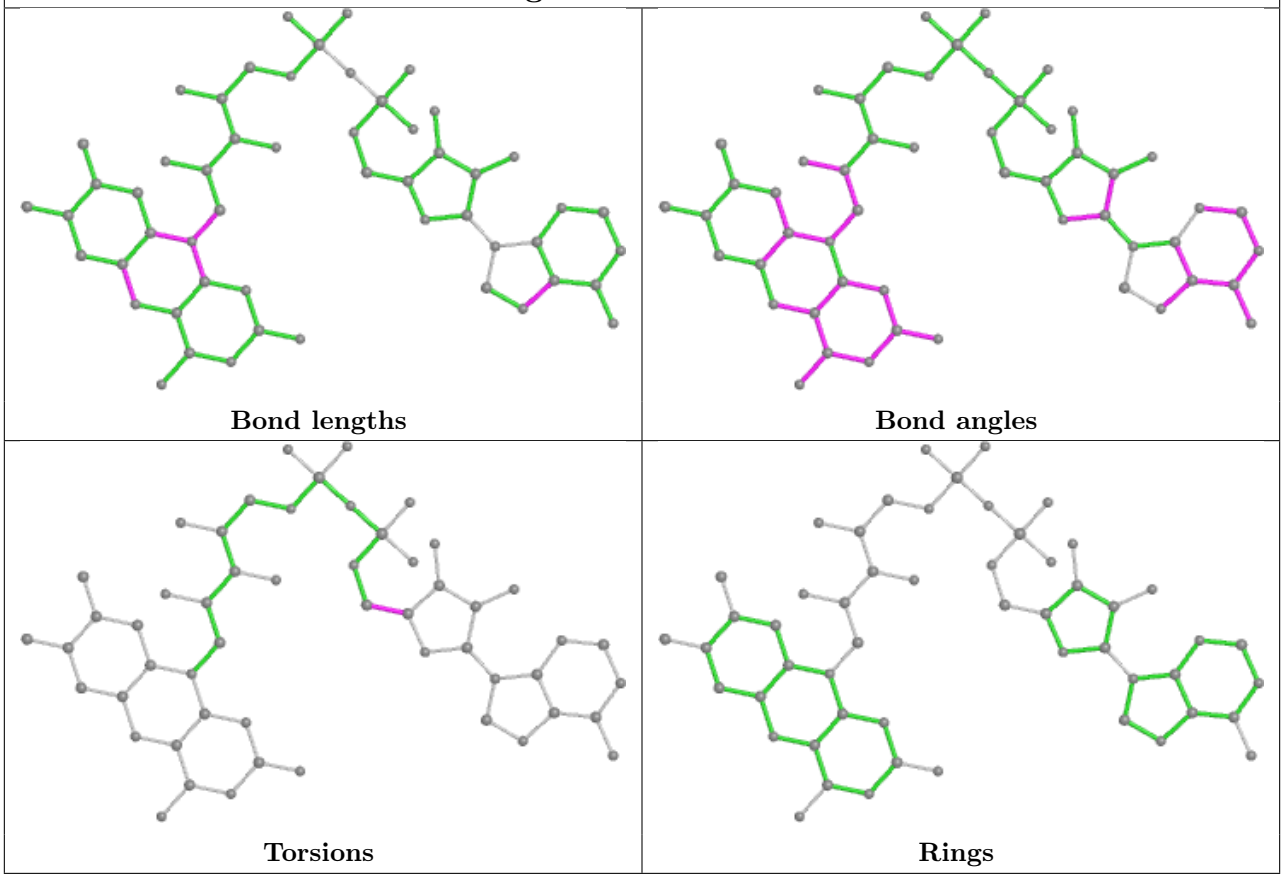


Torsions



Rings

Ligand FAD A 480



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	472/477 (98%)	-0.99	0 100 100	6, 26, 63, 89	0
1	B	472/477 (98%)	-0.94	1 (0%) 95 94	6, 28, 63, 90	0
All	All	944/954 (98%)	-0.96	1 (0%) 95 95	6, 27, 63, 90	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

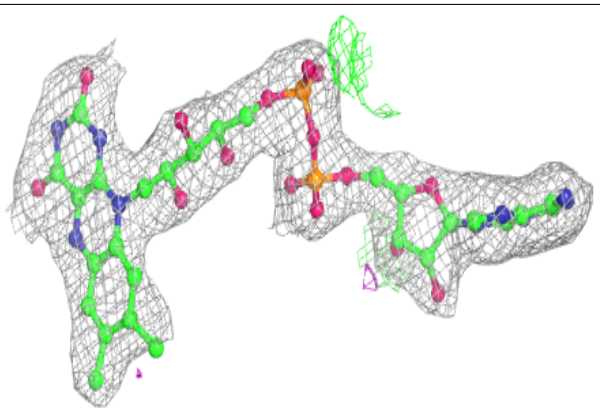
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	A	480	53/53	0.98	0.10	9,23,30,32	0
2	FAD	B	480	53/53	0.98	0.10	10,26,35,37	0

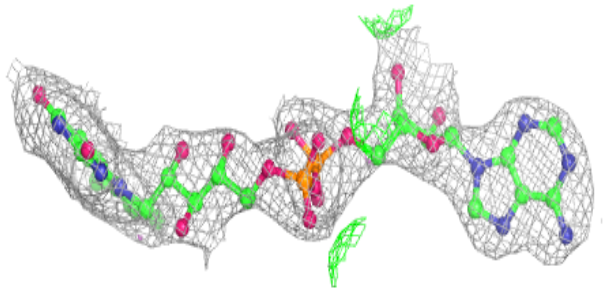
The following is a graphical depiction of the model fit to experimental electron density of all

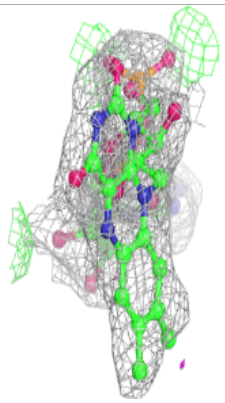
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD A 480:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

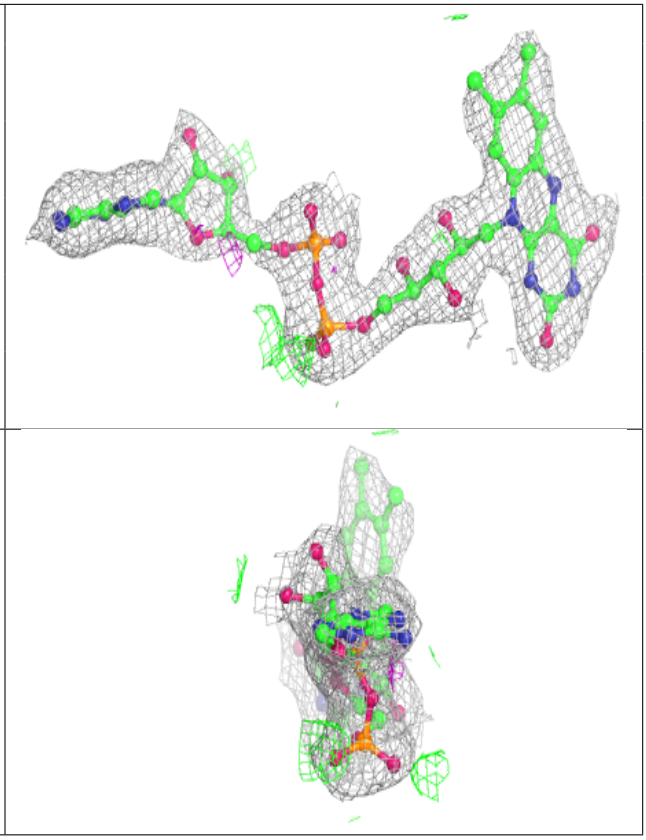






Electron density around FAD B 480:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.